The Effect of Inclusions on Phase Transformations in Dynamically Driven Plates

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Processing techniques, such as hot rolling, may result in the formation of high-aspect ratio inclusions or impurities within the material microstructure. These elongated and aligned inclusions are one source of material anisotropy. Although low in concentration, they may have a significant effect on the material behavior, resulting in an anisotropic plastic or fracture response. A study of the effect of inclusions on the phase transformation characteristics of a dynamically driven matrix material was considered.

The development of predictive material models can expedite the analysis of engineering systems and assist in the interpretation of experimental data. Many heterogeneous materials contain constituents that undergo phase transformations. A few examples are metal matrix composites, high-explosive materials, and alloys that are used in armor designs. In heterogeneous materials, details of the microstructure have a direct effect on the macromechanical response of the material. Consequently, it is important to include the effects of the microstructure when modeling composite materials. However, the length scales that are necessary to model the details of the composite microstructure are much smaller than those of the engineering structure. Therefore, it is impractical to resolve the microstructure for large-scale simulations. Homogenization techniques that use idealized representations for the microstructure and are computationally robust and efficient provide a viable compromise. The generalized method of cells (GMC) is one such technique, which has demonstrated versatility and has been applied to numerous applications.

In dynamically driven structures, there are a number of characteristic time as well as length scales that must be considered. For example, the deformation rate characteristics of the material must be included to accurately model the material response to high-rate loading scenarios. Also, in materials that exhibit solid-solid phase transformations, the kinetics of the transformation process must be addressed. These processes are evident in plate impact experiments. Distinct signatures of rate-dependent plasticity and of the phase transformation are obtained from the measured velocity history on the back surface of the plate.

We developed a macromechanical model for the thermomechanical deformation of heterogeneous materials, which includes the effects of plasticity and phase transformations of its constituents. The model does not resolve the details of the transformation process. Instead, the evolution of the transformation process is addressed by tracking the mass fractions of each phase within the constituents. Each phase is allowed to have distinct material properties. Free energies for each phase, which are derived from ab initio calculations coupled with experimental data, are used. These free energies provide the constitutive response of the constituents. The kinetics of the phase transformation are also expressed in terms of differences of the free energies of the transforming phases.

One example, which illustrates the utility of the homogenization-phase transition (GMC-PT) analysis, considers situations where the phase transformation occurs nonuniformly at the microlevel. This example is different from heterogeneous nucleation and growth phenomena where regions of transforming material begin at a nucleation site and spread outward until the entire material is transformed. Indeed in Fe, using diamond anvil cell (DAC) hydrostatic experiments, it was observed that in addition to the standard nucleation and growth behavior, microscopically small independent areas in the Fe transformed simultaneously. This resulted in a mottled transformation surface as measured by X-ray diffraction and high-pressure light metallographic techniques. To simulate this behavior, a small concentration of Fe was forced to remain in the α-phase, while the remaining subcells were allowed to transform. The effects on the velocity profile then were calculated. For impact velocities of 0.9916 and 1.567 km/s, the calculated velocity profiles are shown in the Fig. 1. Regions of transformation-prohibited Fe (i.e., the impurities) up to 30 volume percent are shown. For the low velocity simulation, while the transformation plateau is reduced, it remains clearly visible even up to a 30 percent impurity level. However, at the higher velocity, an impurity concentration of 30 percent is sufficient to nearly remove the appearance of the phase transformation in the calculated velocity profile.

A second example considered the case where regions of the Fe system were oxidized resulting in iron-oxide (Fe_2O_3) inclusions. The addition of oxygen is known to suppress any phase transformations to higher values of pressure than those probed in the simulations. This is evident from a phase diagram for Fe_2O_3. The second example provides velocity profiles for Fe containing 10 percent Fe_2O_3. To illustrate the flexibility of the GMC-PT analysis, Fe_2O_3 inclusions with aspect ratios of approximately 3 were used in the simulations. The effects of adding 10 percent Fe_2O_3 inclusions to the Fe are shown in Fig. 2. Recall that only the Fe subcells are allowed to transform from α to ε. The Fe_2O_3 elastic bulk and shear moduli are taken from the literature. Values of 98 and 93 GPa were used for the bulk and shear moduli, respectively. It is noted that the bulk modulus of the Fe_2O_3 inclusions is substantially less than for pure Fe. In this example, Fe_2O_3 is modeled as a linear elastic material. Clearly, a full equation of state would provide more representative simulations. For this example, studying the single impact velocity of 0.9916 km/s suffices. The velocity profiles for pure Fe and for 10 % nontransforming inclusions are provided in Fig. 2. Two orientations of Fe_2O_3 inclusions, each having an aspect ratio of 3, are simulated. One orientation has the long-axis of the inclusion aligned with the strain axis of the plate impact simulation. The other simulation has the inclusion aligned perpendicular to the strain axis.

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Citations

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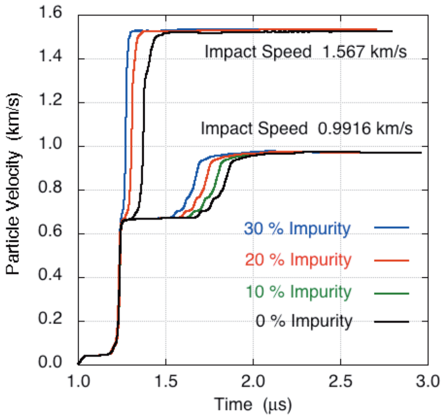

Fig. 1. Theoretical particle velocity profiles for a heterogeneous system where small regions of the Fe phase transformation are suppressed.

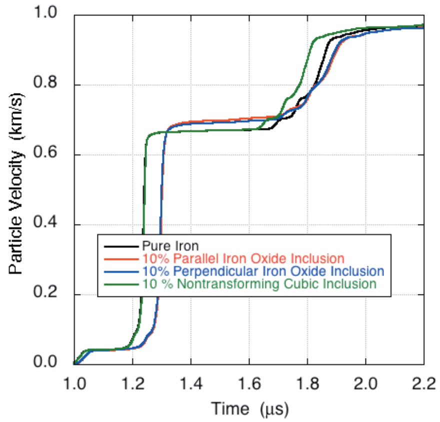

Fig. 2. Theoretical particle velocity profiles for a heterogeneous system containing pure Fe and Fe_2O_3 inclusions.

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